

## Transferred hyperfine interactions for Yb<sup>3+</sup> ions in CsCa F 3 and Cs<sub>2</sub> NaY F6 single crystals: Experimental and ab initio study

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### Abstract

The results of an electron-nuclear double resonance study of the cubic paramagnetic Yb<sup>3+</sup> center in Cs<sub>2</sub> NaY F6 and CsCa F3 single crystals are presented. The values and signs of the transferred hyperfine interaction (THFI) parameters for several neighboring shells are determined. It is found that the relevant parameters for the two studied matrices differ, in spite of the fact that the nearest environment of the rare earth ion is nearly identical. A first-principles theoretical analysis is performed for the THFI parameters of the first coordination shell of F-ions. Several mechanisms of metal ion-ligand coupling are considered and it is found that one of them, ligand polarization, explains the difference observed for the THFI parameters in Cs<sub>2</sub> NaY F6 and CsCa F3. © 2009 The American Physical Society.

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